Topological crystalline insulator transition and spin texture in (Pb,Sn,Mn)Se

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Pb_{1-x}Sn_xSe substitutional alloy is the member of new class of quantum materials – topological crystalline insulators (TCIs) [1]. The topological order is protected by (110) mirror symmetry of the rock-salt crystal structure. This phase is manifested by gapless Dirac-like surface states observed upon inversion in band structure and exhibits specific helical spin texture [2, 3]. In these materials the topological non-trivial state with opposite parity in band structure for high symmetry planes is observed for bulk as well as layered materials [4] and can be controlled by pressure [5], temperature or change of chemical composition [3]. In this work we verify possibility of controlling the TCI transition by band gap engineering via incorporation of manganese ions into host matrix. Previous studies of Pb_{1-x-y}Sn_xMn_ySe showed dE_g/dy equal to 30 meV per at.% of Mn [6]. The second crucial point was verification of protection of the helical spin texture in presence of magnetic ions.

Bulk monocrystals of $Pb_{1-x-y}Sn_xMn_ySe$ with $0.28 \le x \le 0.385$ and $y \le 0.022$ were grown by the Bridgman method. The crystalline quality, lattice parameter and chemical composition were studied by x-ray diffraction and energy-dispersive x-ray spectroscopy. In very diluted regime of the manganese ions (v=0.0003) the electron paramagnetic resonance proved that the Mn ions are in 2+ charge state with spin-only S=5/2 local magnetic moment, hence they are built in cation sublattice positions. For purpose to verify our goals we used freshly cleaved (001)-oriented crystals for both angle-resolved and spin-resolved photoemission spectroscopy at 9 K – 300 K and 65 K, respectively. Analysis of the temperature evolution of band structure for whole studied set of samples shows that the TCI transition appears at lower temperatures with respect to $Pb_{1-x}Sn_xSe$. We found that the $dE_e/dT \approx 50 \text{ meV/K}$ is independent on Mn content and does not change for both trivial and TCI states. Studies of spin texture at TCI state were carried out on the sample with very high Sn content (x=0.385 and y=0.01). Spin resolved spectra taken at both sides of X-bar point of surface Brillouin zone exhibit change of spin polarization. This result is analogous to spin texture obtained for Pb_{1-x}Sn_xSe samples [6] and provides clear evidence that magnetic ions in the crystal matrix of topological crystalline insulators do not destroy TCI order. Finally, we propose phase diagram for Pb_{1-x-v}Sn_xMn_vSe crystals as guideline for further works on TCI band gap engineering.

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